

07-05-00

A
PTO/SB/05 (2/98)Approved for use through 09/30/2000. OMB 0651-0032
Patent and Trademark Office: U.S. DEPARTMENT OF COMMERCEPlease type a plus sign (+) inside this box →

Under the Paperwork Reduction Act of 1995, no persons are required to respond to a collection of information unless it displays a valid OMB control number.

UTILITY PATENT APPLICATION TRANSMITTAL

(Only for new nonprovisional applications under 37 C.F.R. § 1.53(b))

Attorney Docket No. LAM-P0629

First Inventor or Application Identifier David Cooperberg, et al.

Title Method and Apparatus to Calibrate..

Express Mail Label No. EL575423001US

APPLICATION ELEMENTS

See MPEP chapter 600 concerning utility patent application contents.

1. * Fee Transmittal Form (e.g., PTO/SB/17)
(Submit an original and a duplicate for fee processing)
2. Specification [Total Pages 33]
(preferred arrangement set forth below)
 - Descriptive title of the Invention
 - Cross References to Related Applications
 - Statement Regarding Fed sponsored R & D
 - Reference to Microfiche Appendix
 - Background of the Invention
 - Brief Summary of the Invention
 - Brief Description of the Drawings (if filed)
 - Detailed Description
 - Claim(s)
 - Abstract of the Disclosure
3. Drawing(s) (35 U.S.C. 113) [Total Sheets 5]
4. Oath or Declaration [Total Pages]
 - a. Newly executed (original or copy)
 - b. Copy from a prior application (37 C.F.R. § 1.63(d))
(for continuation/divisional with Box 17 completed)
[Note Box 5 below]
 - i. DELETION OF INVENTOR(S)
Signed statement attached deleting inventor(s) named in the prior application, see 37 C.F.R. §§ 1.63(d)(2) and 1.33(b).
5. Incorporation By Reference (useable if Box 4b is checked)
The entire disclosure of the prior application, from which a copy of the oath or declaration is supplied under Box 4b, is considered to be part of the disclosure of the accompanying application and is hereby incorporated by reference therein.

ADDRESS TO: Assistant Commissioner for Patents
Box Patent Application
Washington, DC 20231

6. Microfiche Computer Program (Appendix)
7. Nucleotide and/or Amino Acid Sequence Submission
(if applicable, all necessary)
 - a. Computer Readable Copy
 - b. Paper Copy (identical to computer copy)
 - c. Statement verifying identity of above copies

ACCOMPANYING APPLICATION PARTS

8. Assignment Papers (cover sheet & document(s))
9. 37 C.F.R. §3.73(b) Statement
(when there is an assignee) Power of Attorney
10. English Translation Document (if applicable)
11. Information Disclosure Statement (IDS)/PTO-1449 Copies of IDS Citations
12. Preliminary Amendment
13. Return Receipt Postcard (MPEP 503)
(Should be specifically itemized)
14. * Small Entity Statement(s) Statement filed in prior application, (PTO/SB/09-12) Status still proper and desired
15. Certified Copy of Priority Document(s)
(if foreign priority is claimed)
16. Other: ..Transmittal Letter.....

* NOTE FOR ITEMS 1 & 14: IN ORDER TO BE ENTITLED TO PAY SMALL ENTITY FEES, A SMALL ENTITY STATEMENT IS REQUIRED (37 C.F.R. § 1.27), EXCEPT IF ONE FILED IN A PRIOR APPLICATION IS RELIED UPON (37 C.F.R. § 1.28).

17. If a CONTINUING APPLICATION, check appropriate box, and supply the requisite information below and in a preliminary amendment:

 Continuation Divisional Continuation-in-part (CIP)

of prior application No: _____ / _____

Prior application information: Examiner _____

Group / Art Unit: _____

18. CORRESPONDENCE ADDRESS

Customer Number or Bar Code Label
(Insert Customer No. or Attach bar code label here)

or Correspondence address below

Name	David B. Ritchie					
	D'Alessandro & Ritchie					
Address	P.O. Box 640640					
	City		San Jose	State	CA	Zip Code
Country	USA	Telephone	408-441-1100		Fax	408-441-8400

Name (Print/Type)	David B. Ritchie		Registration No. (Attorney/Agent)	31,562
Signature			Date	6/30/2000

Burden Hour Statement: This form is estimated to take 0.2 hours to complete. Time will vary depending upon the needs of the individual case. Any comments on the amount of time you are required to complete this form should be sent to the Chief Information Officer, Patent and Trademark Office, Washington, DC 20231. DO NOT SEND FEES OR COMPLETED FORMS TO THIS ADDRESS. SEND TO: Assistant Commissioner for Patents, Box Patent Application, Washington, DC 20231.

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re Application of: } Art Unit:
 Cooperberg, et al. } Examiner:
 Serial No. [Not yet assigned] }
 Filed: June 30, 2000 }
 For: METHOD AND APPARATUS TO }
 CALIBRATE A SEMI-EMPIRICAL }
 PROCESS SIMULATOR }

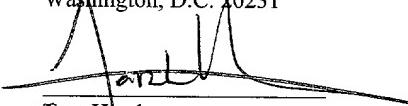
CERTIFICATE OF MAILING

"Express Mail" mailing label no: EL575423001US

Date of Deposit: June 30, 2000

I hereby certify that this correspondence is being deposited with the United States Postal Service "Express Mail Post Office to Addressee" service under 37 CFR 1.10 on the date indicated above and is addressed to:

Box Patent Application
 Assistant Commissioner for Patents
 Washington, D.C. 20231



Tara Hayden

TRANSMITTAL LETTER

Honorable Assistant Commissioner
 for Patents
 Box Patent Application
 Washington, D.C. 20231

Dear Sir:

Enclosed for filing please find the patent application for an invention entitled,
 "METHOD AND APPARATUS TO CALIBRATE A SEMI-EMPIRICAL PROCESS
 SIMULATOR", filed on behalf of LAM Research Corporation, assignee from inventors
 David Cooperberg, Richard A. Gottscho, and Vahid Vahedi, including Utility Patent

Application Transmittal, 25 pages of specification, 7 pages of claims, 5 sheets of drawing figures, and one page of Abstract.

The attorney's Docket Number is LAM-P0629.

Kindly address all communications regarding this application to:

David B. Ritchie
D'Alessandro & Ritchie
P.O. Box 640640
San Jose, CA 95164-0640
Telephone (408) 441-1100

No fee is being paid at this time.

Respectfully submitted,
D'ALESSANDRO & RITCHIE



David B. Ritchie
Reg. No. 31,562

Dated: June 30, 2000

D'Alessandro & Ritchie
P.O. Box 640640
San Jose, CA 95164-0640
(408) 441-1100

This application is submitted in the names of inventors David Cooperberg, Richard A. Gottscho, and Vahid Vahedi, both assignors to Lam Research Corporation, a Delaware Corporation.

5

TITLE OF INVENTION

**METHOD AND APPARATUS TO CALIBRATE A SEMI-EMPIRICAL
PROCESS SIMULATOR**

CROSS-REFERENCE TO RELATED APPLICATIONS

- 10 This is a continuation-in-part of U.S. Patent Application Serial No. 09/033,997, filed March 3, 1998 in the names of inventors Maria E. Barone, Richard A. Gottscho, and Vahid Vahedi and commonly assigned herewith. It is also related to Applications of a semi-empirical physically based profile simulator, Enhanced process and profile simulator algorithms filed in common date herewith.

15

BACKGROUND OF THE INVENTION

Field of the Invention

- This invention relates to plasma processing of semiconductor devices. In particular, this invention provides a method and apparatus to calibrate a semi-
20 empirical process simulator for predicting the surface profile and the etch or deposition rates that a given plasma process will create.

Background Art

Various forms of processing with ionized gases, such as plasma etching and reactive ion etching, are increasing in importance particularly in the area of semiconductor device manufacturing. Of particular interest are the devices used in

5 the etching process. FIG. 1A illustrates a conventional inductively coupled plasma etching system 100 that may be used in the processing and fabrication of semiconductor devices. Inductively coupled plasma processing system 100 includes a plasma reactor 102 having a plasma chamber 104 therein. A transformer coupled power (TCP) controller 106 and a bias power controller 108
10 respectively control a TCP power supply 110 and a bias power supply 112 influencing the plasma created within plasma chamber 104.

TCP power controller 106 sets a set point for TCP power supply 110 configured to supply a radio frequency (RF) signal, tuned by a TCP match network 114, to a TCP coil 116 located near plasma chamber 104. A RF
15 transparent window 118 is typically provided to separate TCP coil 116 from plasma chamber 104 while allowing energy to pass from TCP coil 116 to plasma chamber 104.

Bias power controller 108 sets a set point for bias power supply 112 configured to supply a RF signal, tuned by a bias match network 120, to an
20 electrode 122 located within the plasma reactor 104 creating a direct current (DC) bias above electrode 122 which is adapted to receive a substrate 124, such as a semi-conductor wafer, being processed.

A gas supply mechanism 126, such as a pendulum control valve, typically supplies the proper chemistry required for the manufacturing process to the interior of plasma reactor 104. A gas exhaust mechanism 128 removes particles from within plasma chamber 104 and maintains a particular pressure within

5 plasma chamber 104. A pressure controller 130 controls both gas supply mechanism 126 and gas exhaust mechanism 128.

A temperature controller 134 controls the temperature of plasma chamber 104 to a selected temperature setpoint using heaters 136, such as heating cartridges, around plasma chamber 104.

10 In plasma chamber 104, substrate etching is achieved by exposing substrate 104 to ionized gas compounds (plasma) under vacuum. The etching process starts when the gases are conveyed into plasma chamber 104. The RF power delivered by TCP coil 116 and tuned by TCP match network 110 ionizes the gases. The RF power, delivered by electrode 122 and tuned by bias match network 120, induces a

15 DC bias on substrate 124 to control the direction and energy of ion bombardment of substrate 124. During the etching process, the plasma reacts chemically with the surface of substrate 124 to remove material not covered by a photoresistive mask.

Input parameters such as plasma reactor settings are of fundamental importance in plasma processing. The amount of actual TCP power, bias power,

20 gas pressure, gas temperature, and gas flow within plasma chamber 104 greatly affects the process conditions. Significant variance in actual power delivered to plasma chamber 104 may unexpectedly change the anticipated value of other

process variable parameters such as neutral and ionized particle density, temperature, and etch rate.

Traditionally, a suite of values of these input parameters suitable for creating a given set of device features has been determined by trial and error.

- 5 Development of a single process by this empirical approach is costly and time-consuming, requiring treatment of several patterned wafers and subsequent study of the resulting profiles by scanning electron microscopy. Because of the unpredictable way a small change in one input parameter may affect the profile, any modification of the layout--for example, in device dimension, pattern density
- 10 on the wafer or change in total open area--from one application to another, has often necessitated redevelopment of the process, with the attendant outlay of resources.

- Recent advances in device fabrication technology are rendering this approach even more onerous. Decreasing feature sizes demand tighter tolerances
- 15 on feature dimensions and morphologies, so that the number of trials required to optimize a given process is increasing. The acceleration of wafer diameter growth and the complete redesign of the process involved with an incremental change in diameter have increased the number of times this empirical process must be repeated. The increasing use of devices tailor-made to a specific application also
- 20 increases the amount of development and optimization activity required.

An alternative, computational approach would derive input parameters from a complete physical description of a plasma process including a plasma

model for describing the coupling between the macroscopic input parameters and the macroscopic fluxes, concentrations and energy distributions of the various species in the plasma; and a profile simulator for determining atomistically from the macroscopic fluxes the resulting etch or deposition rate along the wafer surface

- 5 and calculating the profile evolution therefrom. Ideally, such a physical description of plasma etching and deposition processes would enable the *ab initio* selection of the macroscopic input parameters appropriate for generating a desired profile on the substrate, eliminating the need for expensive and time-consuming test sequences.

- 10 Research in this field has done much to elucidate mechanisms at work in plasma processes, and thus has contributed scaling laws that could frame a physical description. However, notwithstanding the availability of computational means sufficiently powerful to perform the necessary calculations based on known scaling laws, the implementation of such an *ab initio* approach has been limited by
15 lack of data. For example, the manner in which the values of some coefficients in these laws depend on the particulars of a given process is unknown as yet. In some investigations, determination of the value of such a scaling coefficient consistent with a plasma process defined by a given set of input parameters has been done by comparing a finished profile, created by applying that process, with
20 a simulated profile including one or more of these coefficients as adjustable parameters. Such hindsight evaluation may promote understanding a given coefficient's role in scaling law, but it has not afforded the ability to predict profile

evolution for any process defined by a set of input parameters differing from the set used in the experimental process used to derive the value of that coefficient.

Thus, there is a need for a method for calibrating a semi-empirical process simulator for predicting the surface profiles and the etch or deposition rates that a

5 given plasma process will create.

SUMMARY OF THE INVENTION

A method and apparatus for calibrating a semi-empirical process simulator used to determine process values in a plasma process for creating a desired surface profile on a process substrate includes providing a test model which captures all mechanisms responsible for profile evolution in terms of a set of unknown surface parameters. A set of test conditions is derived for which the profile evolution is governed by only a limited number of parameters. For each set of test conditions, test values are selected and a test substrate is actually subjected to a test process defined by the test values, thereby creating a test surface profile. The test values are used to generate an approximate profile prediction and are adjusted to minimize the discrepancy between the test surface profile and the approximate profile prediction, thereby providing a final model of the profile evolution in terms of the process values.

CLASSIFICATION CODES

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1A is a block diagram illustrating a plasma etching system.

- 5 FIG.1B is a flow chart illustrating a first calibration process in accordance with a specific embodiment of the present invention.

FIG. 2 is a flow chart illustrating a second calibration process in accordance with a specific embodiment of the present invention.

10

FIG. 3 is an elevational cross-sectional diagram depicting surface kinetics in a plasma process according to the Langmuir model.

- 15 FIG. 4 is a system block diagram illustrating a representative hardware environment in accordance with a specific embodiment of the present invention.

DETAILED DESCRIPTION OF A SPECIFIC EMBODIMENTS OF THE
INVENTION

Those of ordinary skill in the art will realize that the following description
5 of the present invention is illustrative only and not in any way limiting. Other
embodiments of the invention will readily suggest themselves to such skilled
persons having the benefit of this disclosure.

A semi-empirical process simulator is a model that seeks to determine the
10 values of input parameters in a plasma process for creating a desired surface
profile on a substrate, such as a semi-conducting wafer. Previous calibration
schemes used in the process simulator relied on fitting the simulation output to test
data gathered near a process window of interest. While useful, this technique is
likely to produce more empirical and less physically based models. An alternative
15 approach to calibration is to design sets of experiments in which the results are
functions of fewer unknown parameters and for which coefficient values can be
derived from best fit to data with greater confidence. The present invention seeks
to improve such calibration process by using models that more faithfully capture
the actual kinetics governing feature evolution and are likely to yield more
20 accurate profile predictions when using reactor settings which may lie outside a
previously calibrated window of operation.

The form of the surface kinetic model for each class of exposed film and class of plasma chemistry may be derived from experimentally observed trends and scalings. Unknown model coefficients however must be calibrated for each specific film and chemistry. A complete surface kinetics model includes equations 5 governing surface coverage and an equation governing etch or deposition rate.

Surface reaction rates for the adsorption, desorption, and surface reactions of active neutral species lead to a determination of surface coverage. The mechanisms determining local etch rate will be functions of the computed surface coverage and the ion and neutral flux distributions incident on a feature surface 10 element. Etch mechanisms include physical sputtering due to energetic particle bombardment, chemical assisted sputtering which additionally depends on the surface concentration of one or more etchant species, and thermal etching dependent only on chemical coverages (and surface temperature). Deposition rate is typically defined by the adsorption rate of depositing neutral species.

15

The general procedure to calibrate a semi-empirical process simulator is illustrated in FIG. 1. Free parameters needed to characterize mechanisms such as thermal etching, ion enhanced etching, physical sputtering, and deposition are determined by performing test processes under conditions where only a limited 20 number of such mechanisms contribute to etch or deposition rates and/or surface profiles. The reduced set of unknown surface parameters can then be determined by best fit to etch rate and/or surface profile data collected under these conditions.

In block 100, a test model which captures all mechanisms responsible for profile evolution in terms of a set of unknown surface parameters is provided. The input parameters include descriptors of the pre-processing state of the substrate

5 ("substrate parameters") and quantities defining the operation of a given plasma reactor during the test process ("reactor parameters"). The substrate parameters may include, for example, gross dimensions of the substrate, the distribution and dimensions of any features on the surface, and the substrate composition. The reactor parameters may include any of: power levels, gas temperature, gas

10 pressure, inlet gas composition, and length of time the substrate is treated by the plasma process.

In block 102, a set of test conditions is derived from a subset of the test model defined in block 100 such that only a limited number of unknown surface

15 parameters contribute to the etch or deposition rates and the surface profiles. Such test conditions is derived by adjusting the value of some of the surface parameters to render their effects negligible on the test processes.

For each set of test conditions defined in block 102, surface model

20 unknown parameter test values are yet to be solved for. In block 104, these unknown parameter test values are isolated by eliminating parameters that do not contribute to etch or deposition rates or feature evolution.

The unknown parameter test values of reactor variables and reactor fixed parameters as selected in block 106, are used in block 108, in which a plasma model, containing a mathematical description of the plasma in terms of the reactor

parameters for the reactor of interest and coefficients of known or empirically

5 determined value, operates to approximately determine the macroscopic properties of the plasma generated by the test process. The plasma model characterizes the species of interest only as belonging to a general class of actors, for example, as being either charged particles, and thus attracted to the substrate by any applied

bias, or neutral species such as gas molecule and excited radicals. Physical

10 models--for example, Maxwell's and Boltzmann's equations--underlying the functional dependence in terms of governing experimental input parameters of such plasma descriptors as particle fluxes, energy, and angular distributions are well known in the art. (See, e.g., Lieberman and Lichtenberg, *Principles of*

Plasma Discharges and Materials Processing, John Wiley, 1994). Much is known

15 in the art about how these descriptors scale with the input parameters, based on such basic physical models in conjunction with experimental data. However, the absolute value of these fluxes or distributions is not known *a priori* for a given process. Any such coefficient in the reactor model whose value is unknown is treated by the calibration as an adjustable parameter or is determined

20 experimentally.

Those macroscopic properties of the plasma can alternatively be determined by measuring the flux distribution at the wafer in a laboratory under the set of test conditions as selected in block 104.

- 5 In block 112, a profile simulator, containing a mathematical model of the time evolution of the substrate surface profile in terms of the substrate parameters, the macroscopic plasma properties, and coefficients of unknown value, uses the results of block 108 and the substrate parameters provided in block 110 to approximately predict the etch or deposition rates and surface profiles on the
10 substrate. In general, such mathematical model includes a local transport model for calculating fluxes arriving at each point along the substrate surface, a site balance model for calculating the resulting local etch and deposition rates, and a surface advancement algorithm. In a presently preferred specific embodiment of the present invention, a well-known Monte Carlo type approach is used for the
15 local transport.

The site balance model is preferably based on a Langmuir-type model of the kinetics of particle-surface interactions. The model characterizes species that remove material from the substrate as etchants and those that deposit material onto the substrate surface as inhibitors. With reference to FIG. 3, Γ_e and Γ_d respectively represent fluxes of etchants and inhibitors arriving at the surface of the substrate
20 300. Both etchants and inhibitors react with the surface when they encounter a vacant site. Etchant and inhibitor species react at the surface with respective open-

field reaction coefficients of S_e and S_d to form etchant site 302 and inhibitor site 304. The overall occupancies of the substrate surface sites resulting from reactions with etchant and inhibitor species are represented respectively by fractions θ_e and θ_d , with the number of vacant sites 306 being equal to $1-\theta_e-\theta_d$.

- 5 Etch products can form and thermally desorb from the surface. Ions arriving at the surface, at flux Γ , can remove etchants that have reacted with the surface by physical sputtering and ion-enhanced etching; arriving ions can also remove inhibitors from the surface by physical sputtering. Taking into account these assumptions and mechanisms, the site balance, in the steady state, for the two
10 types of occupied sites be expressed respectively as

$$\sigma_e d\theta_e/dt = \Gamma_e S_e (1-\theta_d - \theta_e) - \theta_e k_{sl} \Gamma_{ie} - \theta_e k_{el} \Gamma_{ie} k_{th,e} \theta_e \equiv 0 \text{ and}$$

$$\sigma_d d\theta_d/dt = \Gamma_d S_d (1-\theta_d - \theta_e) - \theta_d k_{sl} \Gamma_{ie} \equiv 0,$$

- 15 Wherein k_{el} , k_{sl} , and k_{th} are coefficients, generally of unknown value, associated with the ion-enhanced, physical sputtering and thermal etching mechanisms, respectively. The parameters Γ_{ie} and Γ_{is} are products of ion-enhanced etching and physical sputtering yields, respectively, with ion flux integrated over incident ion energies greater than respective threshold energies, expressed respectively as E_{th}
20 and E_{th} , and over all angles,

$$\Gamma_{ie} = \iint Y_{ie}(\phi, E) \Gamma_1(\phi, E) d\phi dE = \int dE (E^{\frac{1}{2}} - E_{th,e}^{\frac{1}{2}})^{\frac{1}{2}} \int d\phi Y_e(\phi, E) \int_1(\phi, E) \text{ and}$$

$$\Gamma_{is} = \iint Y_{is}(\phi, E) \Gamma_1(\phi, E) d\phi dE = \int dE (E^{\frac{1}{2}} - E_{th,s}^{\frac{1}{2}})^{\frac{1}{2}} \int d\phi Y_s(\phi, E) \int_1(\phi, E).$$

This model assumes that the etch yields are products of angular functions and the square root of ion energy, which dependence has been observed experimentally. However, other scaling laws could be used instead. The yield functions only represent functional dependencies, the absolute magnitudes being

5 lumped into the coefficients k 's along with other constants.

Expressions for θ_e and θ_d can be derived from the steady-state site balance equation on each type of surface present on the substrate, for example the substrate top and trench bottoms and sidewalls. At each point on the surface, the etch rate,

10 ER, can be written:

$$ER = k_{s2} \Gamma_{ls} + \theta_e k_{e2} \Gamma_{ie} + k_{th} \Gamma_e - k_d \Gamma_d S_d (1-\theta_e).$$

The coefficients k_{e2} , k_{s2} , k_d and k_{th} are yield constants associated with physical sputtering, ion-enhanced etching, thermal etching and ion-induced deposition, respectively. Incorporating the expressions for θ_e , θ_d , Γ_{ls} and Γ_{ie} renders the etch

15 rate in terms of the plasma characteristics and the coefficients k , each of which is in principle an adjustable parameter that can be determined by the calibration.

It is also preferred to employ an analytic scheme for surface advancement so that the fine features can be resolved more accurately. One such scheme known in the art and capable of modeling fine feature aspects, such as sharp corners, is

20 the method of characteristics, also known as the shock-front-tracking algorithm.

(See, e.g., S. Hamaguchi, "Modeling of Film Deposition for Microelectronic Applications", *Thin Films*, vol. 22, p. 81, S. Rossnagel, ed. Academic Press, San

Diego, 1996). Another is the level set approach. (See, e.g., J.A. Sethian, *Level Set Methods: Evolving Interfaces in Geometry, Fluid Mechanics, Computer Vision, and Materials Science*, Cambridge University Press 1996). The shock-front-tracking approach models the surface (i.e., the interface layer between vacuum and solid) as a collection of piecewise continuous line segments, for each of which a rate of movement is calculated. The possibility of each segment's advancing or receding along its normal independently of the movement of the other segments allows for multiple potential solutions for the resulting surface. In order to avoid multiple solutions, these analytic schemes model the points between the line segments as shocks (i.e., discontinuities in the slope), and properly track the movement of the shocks.

Thus, the cumulative output of blocks 104 through 112, particularly of the operation of the plasma model in block 108 and the profile simulator in block 112, which together comprise an initial mathematical surface profile model as specified above, generates a quantitative but approximate prediction of the etch or deposition rates and surface profile(s) created by the test process.

In block 114, the test values of the input parameters provided in block 104 are used to provide a test surface profile, created experimentally by subjecting a test substrate to a test process, in the reactor of interest, defined by the test values of the input parameters. The etch or deposition rates and surface profile(s) of the

test substrate are then measured. In block 116, the etch or deposition rates and surface profile(s) of the test substrate are quantitatively compared with the quantitative approximate prediction resulting from block 112. The difference between the test surface profile(s) and/or etch/deposition rates and the

- 5 approximate prediction(s) is evaluated according to some criterion, such as an accuracy of range of 10%, applied in block 116.

In general, on the first pass, in which the approximate prediction(s) is computed using preliminary test values of unknown surface parameters, the residual is not sufficiently small to satisfy the criterion, and the calibration

- 10 procedure advances to block 118, in which the values of the unknown surface parameters are adjusted so as to minimize the discrepancy. The adjusted values are then resubmitted to the profile simulator of block 112 and the plasma model of block 108, for another iteration that render the approximate profile prediction(s) and of the comparison in block 116. Iteration continues until the discrepancy
15 between the test surface profile(s) and the approximate prediction(s) is adequately minimized.

Thus, both block 116 and block 118 effect a calculation of optimum values

of the unknown surface parameters test values appearing in the initial

- 20 mathematical surface profile model. After the surface parameters suitable for the current set of conditions are determined, a different set of conditions in block 104 is selected from block 102 and its respective surface parameters are determined

using the same process of block 104 through block 120 until all surface parameters are determined.

For example, physical sputtering yield, energy scaling, and energy threshold coefficients may be obtained by fitting to etch rate data and final profile

- 5 SEM (Scanning Electron Micrograph) data collected after wafer processing in a chemically inert plasma such an argon discharge with the ion flux and energy distribution to the separately measured or modeled. Coefficients representing thermal etch rate may be obtained by best fit to etch rate data collected under conditions for which there is no energetic ion bombardment. If sufficient gas
- 10 phase reactant density can be achieve the surface will saturate and the dependence of etch rate on adsorption probability can be eliminated leaving saturated etch rate as the only unknown parameter. Patterned features including overhang structures may be etched in order to isolate surface reaction probabilities which determine transport throughout the feature. In order to calibrate models for deposited
- 15 material, deposition and etch rates on blanket or patterned wafers processed under conditions favoring deposition may be collected. Incomplete film stacks may be used to isolate the mechanisms leading to redeposition. For chemically assisted sputtering, also referred to as ion-neutral synergy etching, data may be collected from wafers processed under conditions where the ratio of ion energy flux to
- 20 etchant neutral flux is varied. For large (small) enough ion energy flux to etchant neutral flux ratios the etch rate is dependent only on the etchant flux (incident ion energy flux). Model fits to this etch rate and profile data combined with ion

and/or neutral flux measurements and/or models can be used to determine unknown coefficients including neutral sticking coefficient, neutral desorption and/or recombination rates, average etch product stoichiometry, and yield per incident ion as a function of energy and angle. For all the sets of experiments 5 above subsets of the complete process chemistry may be used to further isolate and calibrate specific reactions.

DRAFT DRAFT DRAFT DRAFT

In one presently alternative specific embodiment, the approximate profile 10 prediction generated by the profile simulator in block 112 comprises a series of frames, each computed after a sufficiently small time increment, and block 114 only compares frames of the approximate profile prediction that correspond to cumulative exposure times roughly equal to the time of the snapshots in the test surface profile. If the test profile includes multiple snapshots at different exposure 15 times and/or at a different test value of one or more input parameters other than time, block 116 compares each test snapshot with the appropriate frame of the profile prediction and the system operates to minimize the residual over the entire pairwise comparison.

As will now be evident to those of ordinary skill in the art, many 20 configurations departing from the procedure shown in FIG. 1 fall within the scope of the invention. For example, FIG. 2 illustrates another specific embodiment in which block 206 combines the plasma model with the unknown parameter test

values and the substrate parameters in a single module. The entire initial mathematical surface profile model may reside in a single module, block 206, rather than being divided into distinct parts 108 (FIG. 1) and 112 (FIG. 1) to deal separately with phenomena acting over different length scales. Alternatively, 5 depending on the nature of the initial mathematical surface profile model and comparison algorithm used, insertion of the test values and preliminary surface parameters into the initial mathematical surface profile model may be delayed until the comparison block.

10 Turning to FIG. 4, which illustrates, in block-diagram form, a hardware system incorporating the invention. As indicated therein, the system includes a system bus 400, over which all system components communicate, a mass storage device (such as a hard disk or optical storage unit) 402 as well as a main system memory 404.

15

 The operation of the illustrated system is directed by a central-processing unit ("CPU") 406. The user interacts with the system using a keyboard 408 and a position-sensing device (e.g., a mouse) 410. The output of either device can be used to designate information or select particular areas of a screen display 412 to 20 direct functions to be performed by the system.

The main memory 404 contains a group of modules that control the operation of CPU 406 and its interaction with the other hardware components. An operating system 414 directs the execution of low-level, basic system functions such as memory allocation, file management and operation of mass storage

- 5 devices 402. At a higher level, an analysis module 416, implemented as a series of stored instructions, directs execution of the primary functions performed by the invention, as discussed below. Instructions defining a user interface 418 allow straightforward interaction over screen display 412. User interface 418 generates words or graphical images on display 412 to prompt action by the user, and
- 10 accepts user commands from keyboard 408 and/or position-sensing device 410.

The main memory 404 also includes one or more database 420, in general containing any of the test or process values of input parameters including input variables, the desired profile, the test surface profile and rough preliminary test values in the plasma model and profile simulator.

15

It must be understood that although the modules of main memory 404 have been described separately, this is for clarity of presentation only; so long as the system performs all necessary functions, it is immaterial how they are distributed within the system and its programming architecture.

20

The test surface profile(s) is produced experimentally, as is well known in the art, by subjecting one or more test substrates to a test process(es) in a plasma

reactor and measuring the resulting surface profile using, for example, scanning electron microscopy. The desired and test surface profiles may be supplied to the hardware system in electronic format or as graphic hardcopy, in which case the image(s) is processed by a digitizer 398 before numerical comparison with the

5 approximate prediction. The digitized profile is sent as bitstreams on the bus 400 to a database 420 of the main memory 404. The test surface profile may be stored in the mass storage device 402 as well as in database 420.

As noted above, execution of the key tasks associated with the present

- 10 invention is directed by analysis module 416, which governs the operation of CPU 406 and controls its interaction with main memory 404 in performing the blocks necessary to provide a final mathematical surface profile model including calibrated optimum test values in the initial surface profile model; and, by further processing based on the final surface profile model and a desired surface profile,
- 15 to determine process values of one or more input variables governing a plasma process sequence appropriate for creating the desired profile on a process substrate; or, by inserting process values of the input variables into the final mathematical model, to predictively calculate a process surface profile to be created on a process substrate by a plasma process sequence defined by the
- 20 process values.

In particular, the hardware system depicted in FIG. 3 may be used to implement the calibration procedure illustrated by FIG. 1 as follows. The input

variable test values selected in block 104, the test values of any fixed input parameter, and the test surface profile created in block 114 and, as needed, the desired surface profile and/or process values of interest are provided to the database 420 so that they are available to the analysis module 416. Alternatively, 5 the module 416 may retrieve any of the test values, rough preliminary values and test surface profile data from the mass storage device 402 or user interface 418 in response to a user command. Or, the rough preliminary values may be determined by the module 416, based on the input variable test values, according to a predetermined algorithm.

10

Turning now to FIG. 1, by executing the plasma modeling and profile simulation of blocks 108 and 112, respectively, the module 416 establishes the initial mathematical surface model predicting the profile created by the test process. In block 116, the module 416 (FIG. 4) accesses the test surface profile 15 and compares it with the initial mathematical surface profile model and evaluates the residual according to some predetermined criterion. If the residual is not sufficiently small, the analysis module 416 uses the results of the comparison to adjust the test values of the plasma model and profile simulator in block 118. The new test values are retained in the database 420 for another iteration of the 20 modeling/simulation and comparison blocks. When the test surface profile and approximate prediction are sufficiently similar, the test values used in that final iteration are stored in the database 420 as the optimum values.

The analysis module uses these optimum values of the input variables for computation of process values, which can be loaded into a plasma reactor for production of a device including the desired profile, or for profile prediction as
5 described above.

It will therefore be seen that the foregoing represents a highly extensible and advantageous approach to plasma processing of semiconductor devices. The terms and expressions employed herein are used as terms of description and not of
10 limitation, and there is no intention, in the use of such terms and expressions, of excluding any equivalents of the features shown and described or portions thereof, but it is recognized that various modifications are possible within the scope of the invention claimed. For example, the various modules of the invention can be implemented on a general-purpose computer using appropriate software
15 instructions, or on a network of computers, or a multiprocessor computer or as hardware circuits, or as mixed hardware-software combinations (wherein, for example, plasma modeling and profile simulation are performed by dedicated hardware components).

20 While embodiments and applications of this invention have been shown and described, it would be apparent to those skilled in the art having the benefit of this disclosure that many more modifications than mentioned above are possible

without departing from the inventive concepts herein. The invention, therefore, is not to be restricted except in the spirit of the appended claims.

CLAIMS

What is claimed is:

1. A method for calibrating a semi-empirical process simulator, said method comprising:
 - 5 deriving a set of test conditions for which a profile evolution is governed only by a limited number of parameters;
 - selecting a plurality of test values for each said set of test conditions;
 - subjecting a test substrate to a test process defined by said plurality of test values, thereby creating a test surface profile;
 - 10 generating an approximate profile prediction from said plurality of test values;
 - adjusting said plurality of test values to minimize a discrepancy between said test surface profile and said approximate profile prediction, thereby solving for said limited number of parameters; and
 - 15 repeating said selecting, subjecting, generating, and adjusting for another said set of test conditions until said plurality of parameters is determined, thereby providing a final model of said profile evolution in terms said plurality of parameters.
-
- 20 2. The method of claim 1, wherein said profile evolution comprises an etch rate, a deposition rate, and a surface profile.

3. The method of claim 1, wherein generating said approximate profile prediction includes using a plurality of preliminary test values.
4. The method of claim 3, wherein said adjusting said plurality of test values includes changing at least one preliminary test value.
5. The method of claim 4, further comprising comparing said test surface profile and said approximate profile prediction.
- 10 6. The method of claim 5, further comprising incorporating at least one changed preliminary test value.
7. The method of claim 1, wherein said semi-empirical process simulator is used to determine a plurality of parameters governing a plasma process for creating a desired surface profile on a process substrate.
- 15 8. The method of claim 7, further comprising generating a plurality of parameters from said final model and said desired surface profile.
- 20 9. The method of claim 1, wherein said semi-empirical process simulator is used to predict a surface profile to be created on a process substrate by a plasma process defined by a plurality of parameters.

10. The method of claim 8, further comprising generating a prediction of said surface profile from said final model and said plurality of parameters.
- 5 11. The method of claim 1, wherein said plurality of parameters comprises: a plurality of unknown substrate parameters and a plurality of unknown reactor parameters.
- 10 12. The method of claim 11, wherein said plurality of unknown substrate parameters comprises: a dimension of a substrate, a substrate composition, and a distribution of a feature on a surface substrate.
- 15 13. The method of claim 11, wherein said plurality of unknown reactor parameters comprises: a power level, a gas temperature, a gas pressure, a gas flow, and a gas composition.
- 20 14. The method of claim 1, wherein said plurality of parameters varies with time.
- 20 15. A method for configuring an apparatus for calibrating a semi-empirical process simulator, the method comprising the steps of:

deriving a set of test conditions for which a profile evolution is governed only by a limited number of parameters;

selecting a plurality of test values for each said set of test conditions;

subjecting a test substrate to a test process defined by said plurality of test

5 values, thereby creating a test surface profile;

generating an approximate profile prediction from said plurality of test values;

adjusting said plurality of test values to minimize a discrepancy between

said test surface profile and said approximate profile prediction, thereby solving

10 for said limited number of parameters; and

repeating said selecting, subjecting, generating, and revising for another said set of test conditions until said plurality of parameters is determined, thereby providing a final model of said profile evolution in terms said plurality of parameters.

15

16. An apparatus for calibrating a semi-empirical process simulator, the apparatus comprising:

a computer memory for storing a desired surface profile;

a computer memory for storing a test surface profile, created by subjecting

20 a test substrate to a test process defined by a respective plurality of parameters;

means for deriving a set of test conditions for which a profile evolution is

governed only by a limited number of parameters;

- means for selecting a plurality of test values for each said set of test conditions;
- means for subjecting a test substrate to a test process defined by said plurality of test values, thereby creating a test surface profile;
- 5 means for generating an approximate profile prediction from said plurality of test values;
- means for revising said plurality of test values to minimize a discrepancy between said test surface profile and said approximate profile prediction, thereby solving for said limited number of parameters; and
- 10 means for repeating said selecting, subjecting, generating, and revising for another said set of test conditions until said plurality of parameters is determined, thereby providing a final model of said profile evolution in terms said plurality of parameters.
- 15 17. The apparatus of claim 16, further comprising a computer memory for storing a preliminary test value, the means for generating an approximate profile description from the initial surface profile model and the respective test value employing the preliminary test value.

18. A program storage device readable by a machine, tangibly embodying a
program of instructions readable by the machine to perform a method for
calibrating a semi-empirical process simulator, the method comprising:
deriving a set of test conditions for which a profile evolution is governed
5 only by a limited number of parameters;
selecting a plurality of test values for each said set of test conditions;
subjecting a test substrate to a test process defined by said plurality of test
values, thereby creating a test surface profile;
generating an approximate profile prediction from said plurality of test
10 values;
adjusting said plurality of test values to minimize a discrepancy between
said test surface profile and said approximate profile prediction, thereby solving
for said limited number of parameters; and
repeating said selecting, subjecting, generating, and adjusting for another
15 said set of test conditions until said plurality of parameters is determined, thereby
providing a final model of said profile evolution in terms said plurality of
parameters.
19. A program storage device readable by a machine, tangibly embodying a
20 program of instructions readable by the machine to perform a method for
configuring an apparatus for calibrating a semi-empirical process simulator,
the method comprising:

deriving a set of test conditions for which a profile evolution is governed only by a limited number of parameters;

selecting a plurality of test values for each said set of test conditions;

subjecting a test substrate to a test process defined by said plurality of test

5 values, thereby creating a test surface profile;

generating an approximate profile prediction from said plurality of test values;

adjusting said plurality of test values to minimize a discrepancy between said test surface profile and said approximate profile prediction, thereby solving

10 for said limited number of parameters; and

repeating said selecting, subjecting, generating, and revising for another said set of test conditions until said plurality of parameters is determined, thereby providing a final model of said profile evolution in terms said plurality of parameters.

ABSTRACT

A method and apparatus for calibrating a semi-empirical process simulator used to determine process values in a plasma process for creating a desired surface

- 5 profile on a process substrate includes providing a test model which captures all mechanisms responsible for profile evolution in terms of a set of unknown surface parameters. A set of test conditions is derived for which the profile evolution is governed by only a limited number of parameters. For each set of test conditions, test values are selected and a test substrate is actually subjected to a test process
- 10 defined by the test values, thereby creating a test surface profile. The test values are used to generate an approximate profile prediction and are adjusted to minimize the discrepancy between the test surface profile and the approximate profile prediction, thereby providing a final model of the profile evolution in terms of the process values.

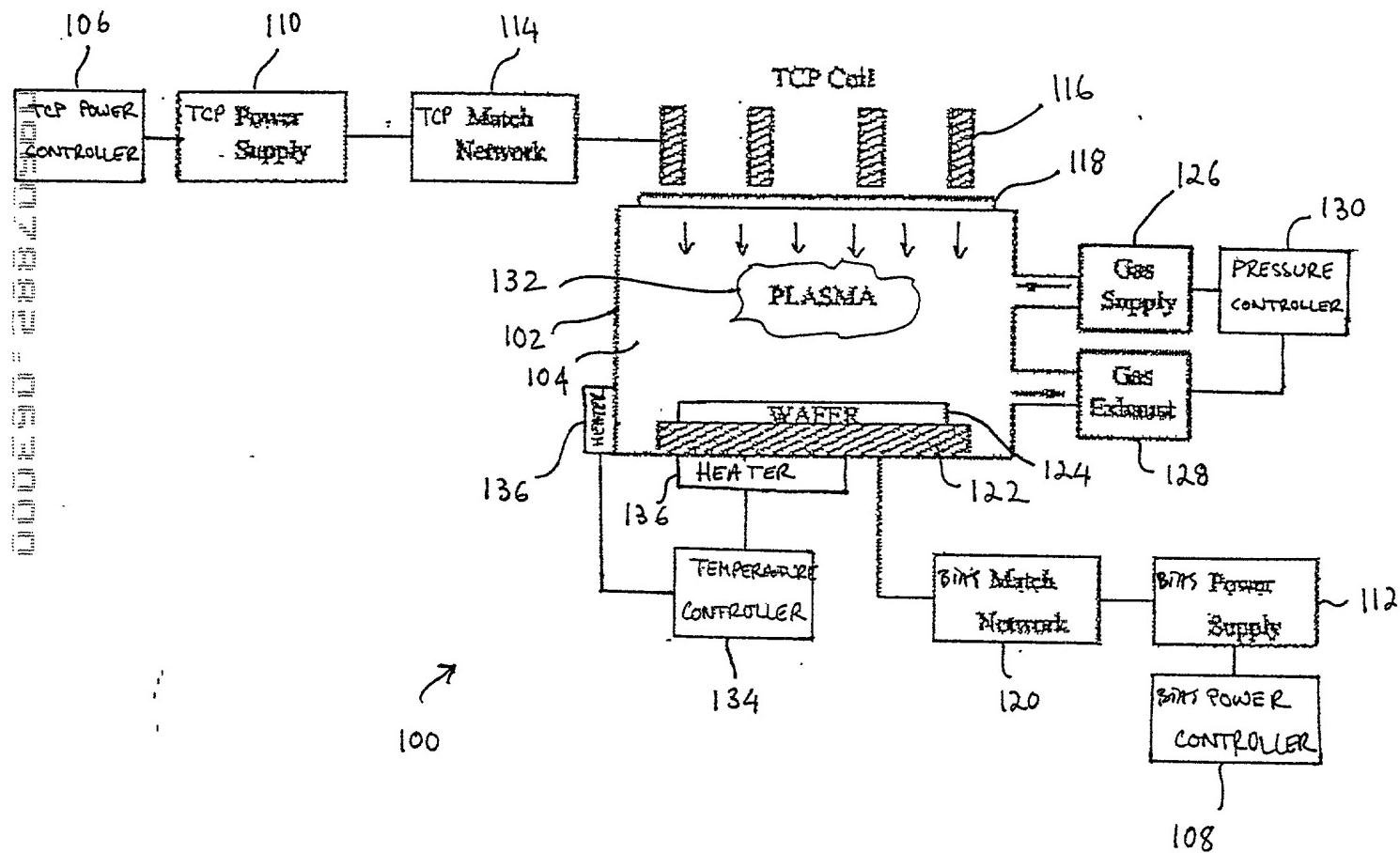


FIG. 1A

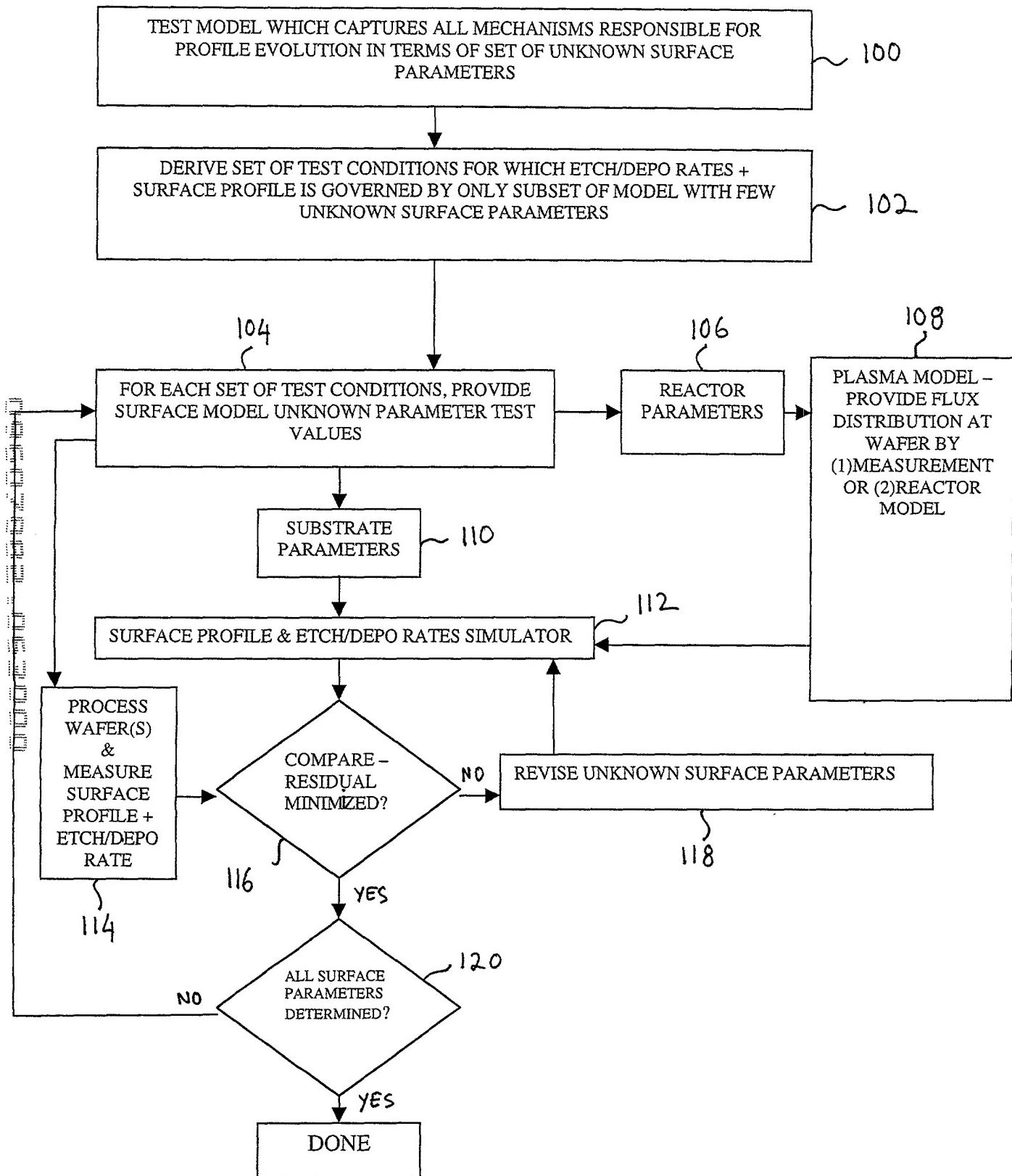


FIG. 1 B

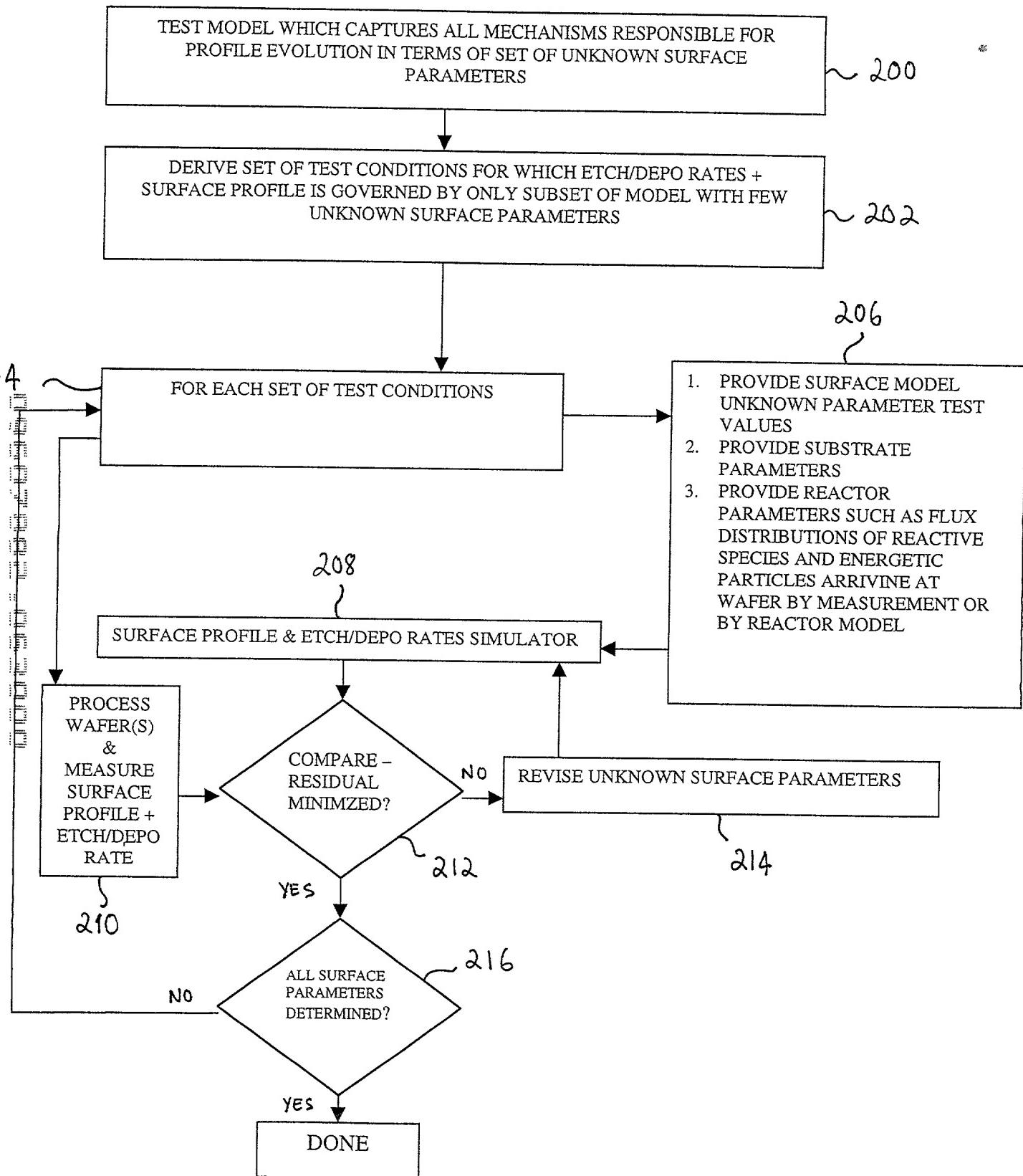


FIG. 2

EL575423001US

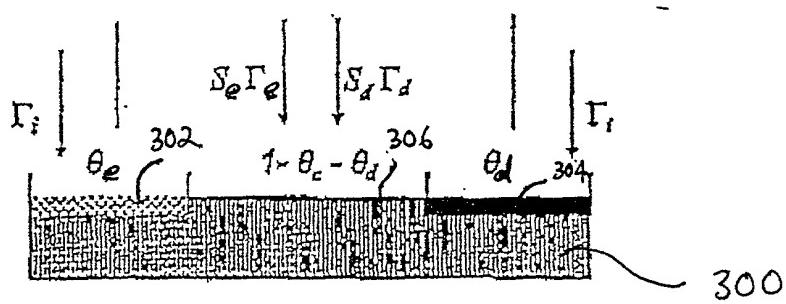


FIG. 3

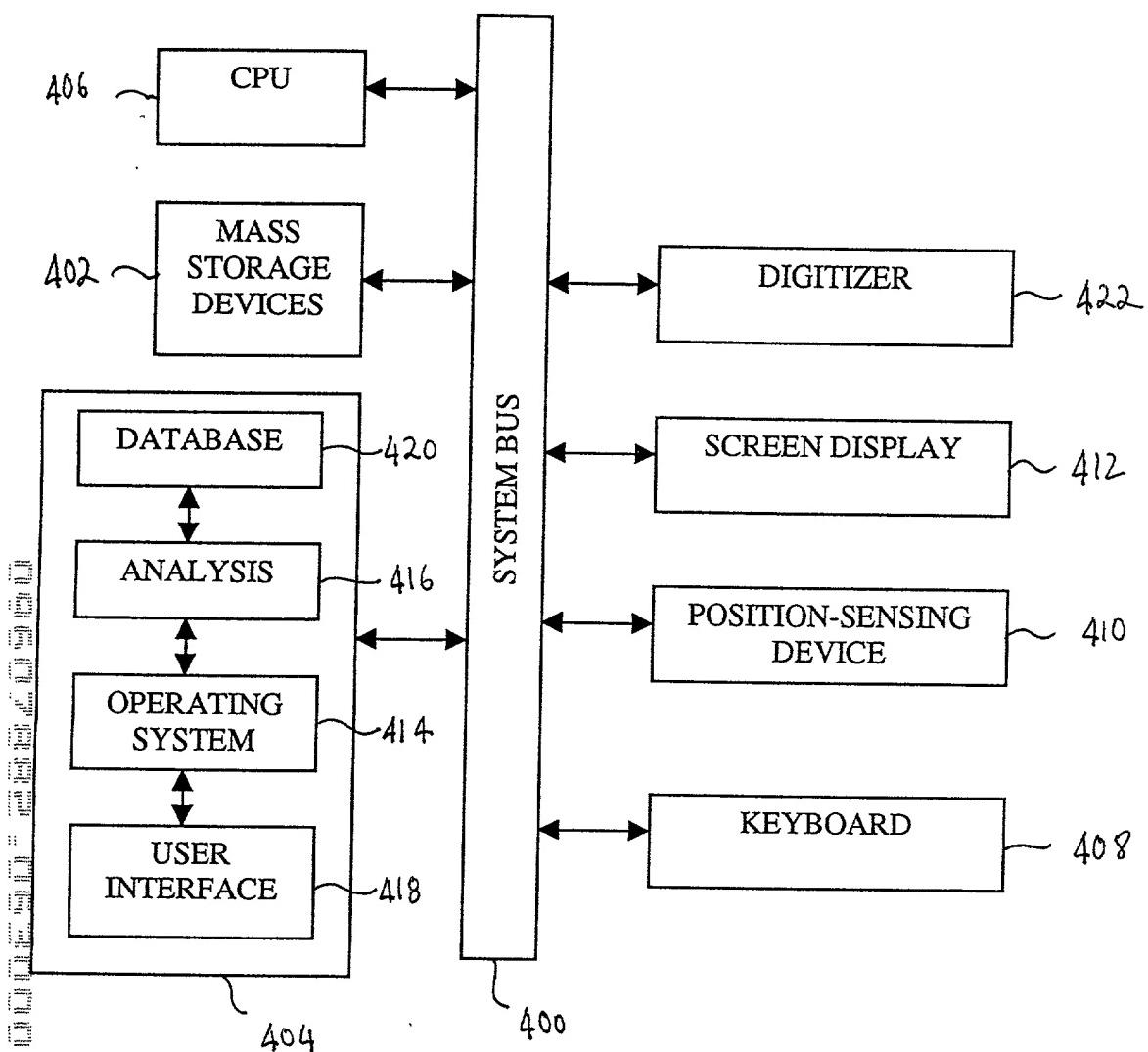


FIG. 4